Large Scale Production Computing Requirements Workshop for Biological and Environmental Research

Yukiko Sekine

Facilities Division

Advanced Scientific Computing Research

May 7 and 8, 2009

Outline of Introduction

- Current approaches to NERSC requirements gathering
- Benefits of SC/HQ-centric requirements gathering for NERSC resources in the context of Programmatic mission needs
- SC/ASCR HPC Facilities and their missions
- NERSC roles in SC HPC services
- Purpose of this workshop

May 7 and 8, 2009

Current Tools for Requirements Gathering for NERSC

Advanced Scientific Computing Research

Document or Action	Owner/Perspective	Frequency
DOE Greenbook – Needs and Directions in High-Performance Computing for the Office of Science, June 2005	NERSC User Group (NUG)/NERSC users	Once every three - five years
NERSC "Visualization Greenbook," October 2002	NUG/NERSC users	Not set
Science-Driven Computing: NERSC's Plan for 2006-2010, May 2005	LBNL NERSC/LBNL NERSC	Once every five years

May 7 and 8, 2009

Assessment of Current Tools

- These documents are very informative.
- They represent either NERSC's User Group's perspective, or LBNL/NERSC Team's perspective.
- *Science-Driven Computing: NERSC's Plan* is the closest to capture SC's needs, and is published once every 5 years.
- Science needs are changing rapidly, and the five-year cycle does not capture the changing needs very effectively.
- We also need more computation-oriented data for NERSC needs than those currently collected using the existing mechanisms.

May 7 and 8, 2009

- SC Program Offices will have direct input on and validation of the requirements and can provide forecasts of needs aligned with mission priorities.

- Requirements gathering workshops in the DC area in the three-year cycle can capture rapidly changing Program-specific needs for NERSC resources better.

- We can document SC programmatic needs for NERSC resources that may not be captured in the five-year cycle planning tools.

- We can leverage the successful structure and approach used for the ESnet requirements workshops.

May 7 and 8, 2009

ASCR HEC Facilities: Providing the Tools

Advanced Scientific Computing Research

- High-Performance Production Computing - National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory
  - Delivers high-end computing to entire DOE SC research community to make world-class scientific discovery
  - Facilitates the improved scalability of applications that will enable them to compete for time at a Leadership Class Facility (LCF)

- Leadership-Class Computing – **Leadership Computing Centers at Argonne National Laboratory and Oak Ridge National Laboratory**
  - Delivers highest computational capability to national and international researchers through peer-reviewed **Innovative and Novel Computational Impact on Theory and Computation (INCITE)** program (80% of resources)

ALCF

WORLD'S FASTEST

ARGONNE LEADERSHIP

JAGUAR

World's Most Powerful Computer. For Science!

The Jaguar system at ORNL provides immense computing power in a balanced, stable system that is allowing scientists and engineers to tackle some of the world's most challenging problems.
—2008, Kelvin Droegemeier, Meteorology Professor, University of Oklahoma.

May 7 and 8, 2009

NERSC Role in ASCR HPC: Keystone

Advanced Scientific Computing Research

- "NERSC continues to be a gold standard of a scientific High Performance Computational Facility." – HPCOA Review August 2008

- Introduction of INCITE in 2004 and LCFs has not reduced needs for NERSC services.

Year	BER Usage	SC Usage
2002	397	3479
2003	526	5413
2004	975	7497
2005	976	7385
2006	2404	16248
2007	6759	68336
2008	20898	146935
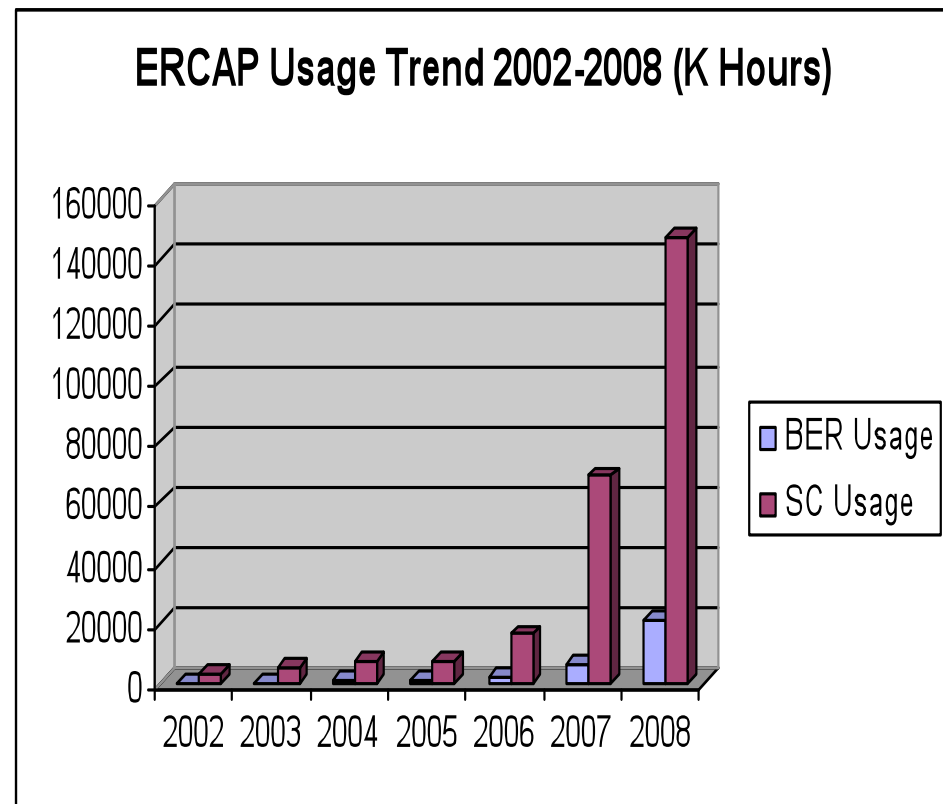
Cray XT-4 Equivalent hours

May 7 and 8, 2009

Purpose of This Workshop

- The goal of this workshop is to accurately characterize the High Performance Computing (HPC) requirements of current and future work funded by the Office of Biological and Environmental Research (BER).

- These requirements will serve as input to the NERSC architecture and planning processes, and will help ensure that NERSC continues to provide world-class support for scientific discovery for DOE scientists and their collaborators.

- The tangible outcome of the workshop will be a document that includes both HPC requirements and a supporting narrative.

May 7 and 8, 2009